

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RJP A. Examiner #: 78680 Date: FEB 25, 2003
 Art Unit: 1913 Phone Number: 272-1104 Serial Number: 10/723,350
 Mail Box and Bldg/Room Location: REM 10 A 24 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

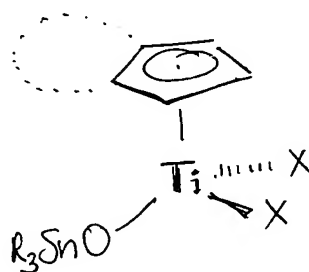
Title of Invention: STANNOXY-SUBSTITUTED METALLOCENE CATALYSTS

Inventors (please provide full names): MARTIN, Joel L. JENSEN, Michael D.
McDANIEL, Max P.

Earliest Priority Filing Date: 11-26-2003

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for compounds having the following minimum structure



SCIENTIFIC REFERENCE BR
 Sci & Tech Inf. Ctr.

FEB 25 RECD

Pat. & T.M. Office

• indenyl, cyclopentadienyl or fluorenyl π -ligand maybe substituted.

• R is allyl, aryl (phenyl)

• Key words which may help

"monocyclopentadienyl"
 "half sandwich" metallocene
 "half metallocene"

"stannyly"
 "stannyloxy"
 "stannoxy"

STAFF USE ONLY

Searcher: Ed
 Searcher Phone #: _____
 Searcher Location: _____
 Date Searcher Picked Up: _____
 Date Completed: 3-6-05
 Searcher Prep & Review Time: _____
 Clerical Prep Time: _____
 Online Time: _____

Type of Search

NA Sequence (#) _____
 AA Sequence (#) _____
 Structure (#) _____
 Bibliographic _____
 Litigation _____
 Fulltext _____
 Patent Family _____
 Other _____

Vendors and cost where applicable

STN _____
 Dialog _____
 Questel/Orbit _____
 Dr.Link _____
 Lexis/Nexis _____
 Sequence Systems _____
 WWW/Internet _____
 Other (specify) _____

CLAIMS

We Claim:

- 5 1. A compound having the following formula:
 $(X^1)(X^2)(X^3)(X^4)M^1$; wherein
 M^1 is selected from titanium, zirconium, or hafnium;
 (X^1) is selected from cyclopentadienyl, indenyl, fluorenyl, substituted
cyclopentadienyl, substituted indenyl, or substituted fluorenyl;
10 each substituent on the substituted cyclopentadienyl, substituted indenyl, or
substituted fluorenyl (X^1) is independently selected from an aliphatic group, an
aromatic group, a cyclic group, a combination of aliphatic and cyclic groups, an
oxygen group, a sulfur group, a nitrogen group, a phosphorus group, an arsenic
group, a carbon group, a silicon group, a germanium group, a tin group, a lead
15 group, a boron group, an aluminum group, an inorganic group, an organometallic
group, or a substituted derivative thereof, any one of which having from 1 to about
20 carbon atoms; a halide; or hydrogen;
 (X^2) is selected from a stannoxy group with the following formula:
 $-OSnR_3$;
20 wherein R is independently selected from alkyl, cycloalkyl, aryl, aralkyl,
substituted alkyl, substituted aryl, or substituted aralkyl, any one of which having
from 1 to about 20 carbon atoms; OR' wherein R' is selected from alkyl, aryl,
aralkyl, substituted alkyl, substituted aryl, or substituted aralkyl, any one of which
having from 1 to about 20 carbon atoms; F; Cl; Br; or I; and
25 (X^3) and (X^4) are independently selected from an aliphatic group, an
aromatic group, a cyclic group, a combination of aliphatic and cyclic groups, an
oxygen group, a sulfur group, a nitrogen group, a phosphorus group, an arsenic
group, a carbon group, a silicon group, a germanium group, a tin group, a lead
group, a boron group, an aluminum group, an inorganic group, an organometallic
30 group, or a substituted derivative thereof, any one of which having from 1 to about
20 carbon atoms; or a halide.

2. The compound of Claim 1, wherein the compound has the following general formula:



5 cycloalkadienyl is selected from cyclopentadienyl, indenyl, fluorenyl, or substituted analogs thereof;

M is selected from Ti, Zr, or Hf;

R is independently selected from substituted or non-substituted alkyl, cycloalkyl, aryl, aralkyl, alkoxide, or aryloxy, any one of which having from 1 to
10 about 20 carbon atoms; F; Cl; Br; or I; and

X is independently selected from F; Cl; Br; I; or a substituted or non-substituted alkyl, cycloalkyl, aryl, aralkyl, alkoxide, or aryloxy, any one of which having from 1 to about 20 carbon atoms.

15 3. The compound of Claim 1, wherein the compound is selected from:

$(\eta^5\text{-cyclopentadienyl})\text{titanium}(\text{triphenylstannoxy})\text{dichloride};$

$(\eta^5\text{-cyclopentadienyl})\text{zirconium}(\text{triphenylstannoxy})\text{dichloride};$

$(\eta^5\text{-cyclopentadienyl})\text{titanium}(\text{trimethylstannoxy})\text{dichloride};$

$(\eta^5\text{-cyclopentadienyl})\text{zirconium}(\text{triethylstannoxy})\text{dichloride};$

20 $(\eta^5\text{-cyclopentadienyl})\text{hafnium}(\text{triphenylstannoxy})\text{dichloride};$

$(\eta^5\text{-cyclopentadienyl})\text{titanium}(\text{tri-n-butylstannoxy})\text{dichloride};$

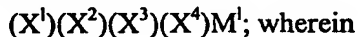
$(\eta^5\text{-cyclopentadienyl})\text{titanium}(\text{triphenylstannoxy})\text{dibromide};$

$(\eta^5\text{-pentamethylcyclopentadienyl})\text{titanium}(\text{triphenylstannoxy})\text{dibromide};$

or

25 $(\eta^5\text{-cyclopentadienyl})\text{titanium}(\text{tributylstannoxy})\text{dibromide}.$

4. A composition of matter comprising a half-sandwich metallocene compound with the following formula:



30 M^1 is selected from titanium, zirconium, or hafnium;

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E FERROCENE/CN

L1 1 S E3
L2 STR 102-54-5

FILE 'REGISTRY' ENTERED AT 15:25:41 ON 06 MAR 2005

L3 0 S L2
L4 STR L2
L5 STR L4
L6 0 S L5
L7 0 S L4
L8 4 S L5 FUL
SAV L8 LEE350/A

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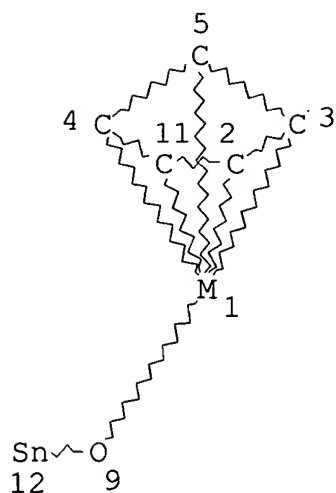
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4 ANSWERS

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L10 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:721207 ZCAPLUS
 DN 132:50061
 ED Entered STN: 12 Nov 1999

TI Synthesis and X-ray crystal structure elucidation of an
organometallic oxide containing Nb and Sn
AU Silva, Rosalice Mendonca; Huffmann, John C.
CS Departamento de Quimica, Universidade Federal de Minas Gerais, Belo
Horizonte, 31270-901, Brazil
SO Polyhedron (1999), 18(22), 2823-2826
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
AB The organometallic oxide $(\eta^5\text{-C}_5\text{H}_5)_2\text{Nb}(\text{Cl})(\mu\text{-O})\text{Sn}(\text{Ph})_2\text{Cl}_2$, 2,
was prep'd. and characterized by spectroscopic methods and elemental
anal. The mol. structure was det'd. by x-ray crystallog. The Nb
atom is in a pseudotetrahedral coordination geometry environment
comprised of the two Cp rings and the Cl and O atoms. The
coordination geometry around the Sn atom is a distorted trigonal
bipyramidal. The det'd. Nb-O bond distance of 1.789(6) Å.
indicates a partial double bonding between Nb and O. Although the
Sn-O bond can be described as a dative bond, it is a very strong
interaction, 2.22(16) Å. The formation of 2 involved the
activation of one of the Sn-Cphenyl bonds of the Sn starting
material. Residual H₂O present in the reaction solvent was the
source of the bridging O in the mol.
ST crystal structure niobium tin oxide complex; mol structure niobium
tin oxide; niobium tin oxide complex prepn structure
IT Crystal structure
Molecular structure
(of a niobium-tin oxide complex)
IT 252990-49-1P
(crystal structure; prepn. and structure of a niobium-tin oxide
complex)
IT 639-58-7, Chlorotriphenylstannane 12793-14-5, Niobocene dichloride
(prepn. and structure of a niobium-tin oxide complex)
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Azevedo, N; J Braz Chem Soc 1998, V9, P279 ZCAPLUS
(2) Chisholm, M; Inorg Chem 1984, V23, P1021 ZCAPLUS
(3) Eaborn, C; J Chem Soc Dalton Trans 1976, P767 ZCAPLUS
(4) Fu, P; J Organomet Chem 1996, V506, P49 ZCAPLUS
(5) Griffith, W; Coord Chem Rev 1970, V5, P459 ZCAPLUS
(6) Holt, M; Chem Rev 1989, V89, P11 ZCAPLUS
(7) Labinger, J; Adv Chem Ser 1979, V167, P149
(8) Lemenovskii, D; J Organomet Chem 1985, V292, P217 ZCAPLUS
(9) Nakamoto, K; Infrared and Raman Spectra 4th ed 1986, P107
(10) Okara, R; J Organomet Chem 1964, V1, P356
(11) Prout, K; Acta Crystallogr Sect B 1974, V30, P2290

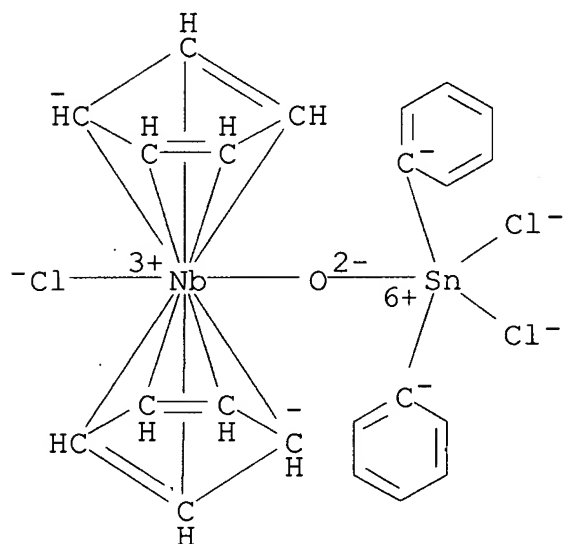
- (12) Rheingold, A; Acta Crystallogr Sect C 1991, V47, P1963
 (13) Silva, R; PhD Thesis Universidade Federal de Minas Gerais 1989
 (14) Skripkin, Y; J Coord Chem 1985, V3, P570
 (15) Steunou, N; Inorg Chem 1998, V37, P910
 (16) Urbanos, F; J Organomet Chem 1984, V276, P185 ZCAPLUS

IT 252990-49-1P

(crystal structure; prepn. and structure of a niobium-tin oxide complex)

RN 252990-49-1 ZCAPLUS

CN Niobium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(dichlorodiphenyltin)-.mu.-oxo-, stereoisomer (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:634252 ZCAPLUS

DN 129:316333

ED Entered STN: 08 Oct 1998

TI Formation of sulfido niobium complexes through C-S bond activation

AU Azevedo, Nelio Pires; Lopes, Antonio Ricardo Giuliani; Silva, Rosalice Mendonca; Speziali, Nivaldo Lucio; Abras, Anuar; Horner, Manfredo; Burrow, Robert Alan

CS Departamento de Quimica, Universidade Federal de Minas Gerais, Belo Horizonte, 31.270-901, Brazil

SO Journal of the Brazilian Chemical Society (1998), 9(3), 279-285
 CODEN: JOCSET; ISSN: 0103-5053

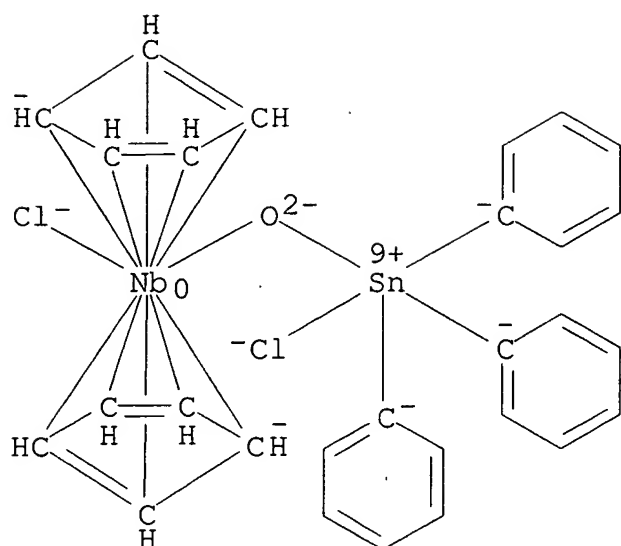
PB Sociedade Brasileira de Quimica

DT Journal

LA English

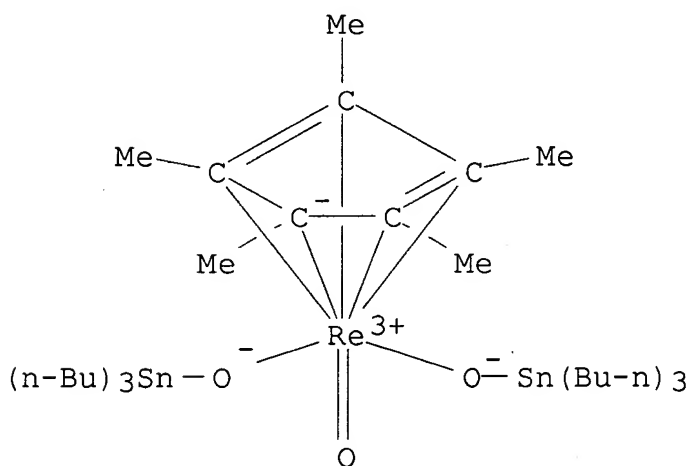
- CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
- AB Upon reacting (.eta.5-C5H5)2NbCl2, .eta.5-C5H5 = Cp, and
(Ph)3Sn(SPh), in THF, [(eta.5-C5H5)2Nb(Cl)(.mu.-S)Sn(Ph)3(Cl)] (1)
and (.eta.5-C5H5)2Nb(S)Cl (2) were obtained. Complexes 1 and 2 were
characterized by IR, 1H-NMR, 13C-NMR, Mossbauer spectroscopies,
elemental anal. as well as by at. absorption. Hydrolysis of 1
yielded the .mu.-oxo species, [(eta.5-C5H5)2Nb(Cl)(.mu.-
O)Sn(Ph)3Cl], which was characterized by IR, 1H-NMR, 13C-NMR and
Mossbauer spectroscopies, elemental anal., at. absorption as well as
by x-ray crystallog. It crystallizes in the space group Pca21 with
a 17.282(3), b 18.122(4), c 17.3269(2) , and Z = 8. Addnl. studies
indicated that the complexes were formed as a result of the
nucleophilic displacement of the Nb-chloride bond by the thiolate
ligand followed by a C-S bond cleavage. The cleavage occurs with an
excess of the thiolate compd. equal to or >2:1.
- ST crystal structure niobium tin oxo bridged; mol structure niobium tin
oxo bridged; niobium sulfido complex prepn hydrolysis; tin niobium
oxo bridged prepn structure; carbon sulfur bond activation
phenylthiostannane niobium
- IT Bond cleavage
(carbon-sulfur; of (phenylthio)triphenylstannane in reactions
with niobium chloro cyclopentadienyl complex)
- IT Reduction, electrochemical
Reduction potential
(of niobium cyclopentadienyl sulfido and niobium-tin
cyclopentadienyl sulfido-bridged complexes)
- IT Crystal structure
Molecular structure
(of niobium-tin cyclopentadienyl chloro Ph oxo-bridged dinuclear
complex)
- IT 1441-22-1, Triphenyl(phenylthio)stannane 12793-14-5,
Dichlorobis(.eta.5-cyclopentadienyl)niobium
(carbon-sulfur bond cleavage in reaction of niobium chloro
cyclopentadienyl complex with triphenyl(phenylthio)stannane)
- IT 139-66-2, Diphenyl sulfide 1064-10-4, Hexaphenyldistannane
(formation from niobium chloro cyclopentadienyl complex with
triphenyl(phenylthio)stannane)
- IT 214785-34-9P
(prepn. and crystal structure of)
- IT 214785-32-7P, Chlorobis(.eta.5-cyclopentadienyl)(thio)niobium
(prepn. and electrochem. of)
- IT 214785-31-6P
(prepn., electrochem. and hydrolysis of)
- RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Adams, R; Organometallics 1992, V11, P2488 ZCAPLUS
(2) Alcock, N; Acta Cryst Section C 1994, P227 ZCAPLUS

- (3) Barbieri, R; J Chem Soc, Dalton Trans 1989, P519 ZCAPLUS
 - (4) Boorman, P; Inorg Chem 1991, V30, P3886 ZCAPLUS
 - (5) Brooker, S; Acta Cryst 1991, VC47, P2527 ZCAPLUS
 - (6) Brunner, H; J Organomet Chem 1990, V381, PC7
 - (7) Cerrada, E; J Organomet Chem 1995, V492, P105 ZCAPLUS
 - (8) Coucovanis, D; Inorg Chem 1994, V33, P3645
 - (9) Darensbourg, M; Organometallics 1989, V8, P1315 ZCAPLUS
 - (10) Douglas, W; J Chem Soc Dalton 1972, P1976
 - (11) Fu, P; J Organomet Chem 1996, V506, P49 ZCAPLUS
 - (12) Green, M; J Chem Soc, Dalton Trans 1991, P1407 ZCAPLUS
 - (13) Griffith, W; Coord Chem Rev 1970, V5, P459 ZCAPLUS
 - (14) Guimaraes, B; Quimica Nova 1995, V18, P329
 - (15) Herrmann, W; Angew Chem Int Ed Engl 1986, V25, P56
 - (16) Holt, M; Chem Rev 1989, V89, P11 ZCAPLUS
 - (17) Kawaguchi, H; J Am Chem Soc 1995, V117, P3885 ZCAPLUS
 - (18) Kawaguchi, H; Organometallics 1997, V16, P307 ZCAPLUS
 - (19) Kayser, F; Organometallics 1994, V13, P4026 ZCAPLUS
 - (20) Kee, T; Coord Chem Rev 1993, V127, P155 ZCAPLUS
 - (21) Mahon, M; J Organomet Chem 1996, V511, P227 ZCAPLUS
 - (22) Mansur, M; Organometallics 1995, V14, P5460
 - (23) Okara, R; J Organomet Chem 1964, V1, P356
 - (24) Okawara, R; Organotin Compounds, Chapter 5 1971, V2 ZCAPLUS
 - (25) Omae, I; Organotin Chemistry, J Organomet Chem Library 21, Chapter 8 1989, P285
 - (26) Osakada, K; Organometallics 1995, V14, P4542 ZCAPLUS
 - (27) Proulx, G; Organometallics 1996, V15, P133 ZCAPLUS
 - (28) Prout, K; Acta Cryst Sect B 1974, V30, P2290
 - (29) Rheingold, A; Acta Cryst 1991, VC47, P1963 ZCAPLUS
 - (30) Riaz, U; J Am Chem Soc 1994, V116, P4357 ZCAPLUS
 - (31) Sheldrich, G; Shelxtl/PC Users Manual 1990
 - (32) Urbanos, F; J Organomet Chem 1984, V276, P185 ZCAPLUS
 - (33) Wilkinson, G; J Chem Soc, Dalton Trans 1980, P1888
- IT 214785-34-9P
(prepn. and crystal structure of)
- RN 214785-34-9 ZCAPLUS
- CN Niobium, chloro(chlorotriphenyltin)bis(.eta.5-2,4-cyclopentadien-1-yl)-.mu.-oxo-, stereoisomer (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1989:574309 ZCAPLUS
 DN 111:174309
 ED Entered STN: 10 Nov 1989
 TI Multiple bonds between Main Group elements and transition metals.
 LXV. Addition of hexamethyldistannane to an organometal oxide with
 cleavage of the tin-tin bond
 AU Herrmann, Wolfgang A.; Marz, Dieter W.
 CS Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed.
 Rep. Ger.
 SO Journal of Organometallic Chemistry (1989), 362(1-2), C5-C7
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA German
 CC 29-11 (Organometallic and Organometalloidal Compounds)
 OS CASREACT 111:174309
 AB A general synthetic route to trialkylstannoxy compds. of the
 organotransition metal series was found, viz. the addn. of
 Me₂SnSnMe₃ to trioxo(.eta.5-pentamethylcyclopentadienyl)rhenium(VII)
 . The reaction occurs with concomitant cleavage of the tin-tin
 bond, and the air-sensitive product oxo(.eta.5-
 pentamethylcyclopentadienyl)bis(trimethylstannoxy)rhenium(V) (I) was
 obtained in 90% yield. The Bu deriv. of I is prepd. analogously.
 ST hexamethyldistannane addn trioxopentamethylcyclopentadienylrhenium;
 rhenium pentamethylcyclopentadienyl trioxide addn
 hexaalkyldistannane; stannoxypentamethylcyclopentadienylrhenium
 oxide; oxopentamethylcyclopentadienylbistrialkylstannoxyrhenium; tin
 tin bond cleavage hexaalkyldistannane; stannoxyrhenium oxo

- cyclopentadienyl
- IT Addition reaction
(of hexaalkyldistannanes with trioxo(pentamethylcyclopentadienyl) rhenium)
- IT Bond cleavage
(tin-tin, in addn. reaction of trioxo(pentamethylcyclopentadienyl) rhenium with hexaalkyldistannanes)
- IT 90695-83-3
(addn. reaction of, with hexamethyl- and hexabutyldistannane)
- IT 661-69-8, Hexamethyldistannane 813-19-4, Hexabutyldistannane
(addn. reaction of, with trioxo(pentamethylcyclopentadienyl) rhenium, tin-tin bond cleavage by)
- IT 123037-83-2P 123060-03-7P
(prepn. of)
- IT 123037-83-2P 123060-03-7P
(prepn. of)
- RN 123037-83-2 ZCAPLUS
- CN Rhenium, oxo[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]bis(tributylhydroxystannanato)- (9CI) (CA INDEX NAME)



- RN 123060-03-7 ZCAPLUS
- CN Rhenium, bis(hydroxytrimethylstannanato)oxo[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

